Ion-Beam induced grain rotation in nanocrystalline alumina

S. Klaumünzer[1,2], M. Bender[1], A. Romanenko[1], D. Severin[1,#]
[1]GSI, Darmstadt, Germany; [2]HZ Berlin, Berlin, Germany

Single crystals of α-alumina (orientation $[11\bar{2}0]$, 15×10×1 mm^3) were bombarded at room temperature with 4.8 MeV/u Au ions. The transformation of the single crystals into nanocrystals was followed by monitoring the $(11\bar{2}0)$-diffraction peak by CuKα-radiation at the in-situ 3-circle-diffractometer at the UNILAC M2-beamline. The ω-circle (incident x-ray beam) and the θ-circle (diffracted beam) define the diffraction plane. The χ-circle enables a sample tilt relative to the diffraction plane; for $\chi = 0$ the sample normal lies in the diffraction plane and coincides with the ion beam direction. During irradiation χ_i was ±45°. X-ray measurements were done by varying χ and $\omega = \theta$ fixed at the Bragg angle θ_B. The single peak originally located at $\chi = 0$ splits with increasing fluence into two peaks, one located at $\chi_1 = 0$, originating from unmodified material at greater specimen depths, and a second one, located at χ_2, resulting from tilted $(11\bar{2}0)$-lattice planes. The tilt angle $\Omega = -\chi_2$ versus fluence is shown in fig. 1. At a fluence of 1×10^{13} Au/cm^2 χ_i has moved from +45° to –45°. The rotation direction also changed its sign. A symmetric Bragg scan at $\chi = \chi_2$ yields the precise position of θ_B and the peak width of the modified alumina. θ_B decreased by about 0.1°, which is attributed to a volume increase by dislocation production. The width of the modified peak is shown in fig. 2. The change in χ_i is not visible in the behavior of the width.

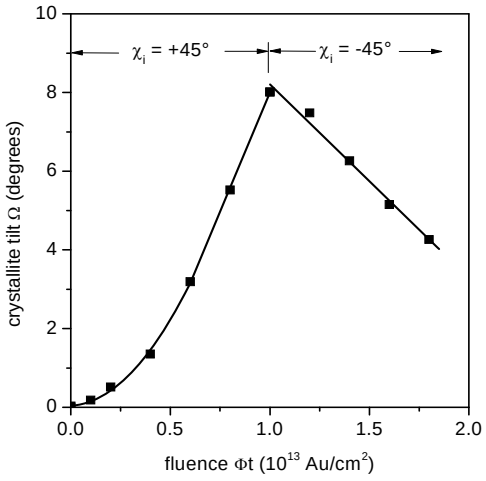

Figure 1: Crystallite tilt Ω versus ion fluence.

Both grain rotation and the square-root dependence of the width (see fig. 2) indicated the action of dislocations. Because the number density of dislocations is of the order of Φt, most of the dislocations are concentrated in newly formed grain boundaries. Thus, at Φt ~10^{12} Au/cm^2 the single crystal is transformed into an aggregate of nanocrystals. The evolution of the grain size is depicted in fig. 3 for two data evaluation strategies.

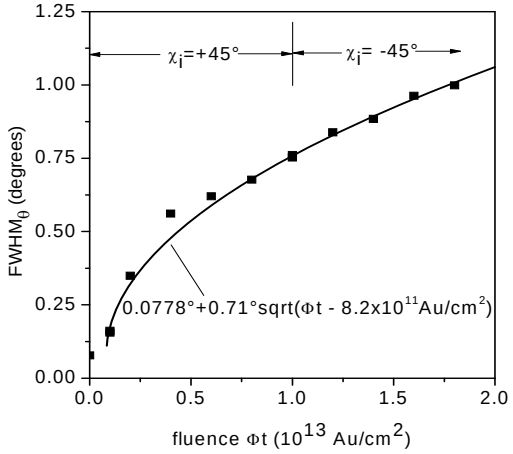

Figure 2: The full width at half maximum FWHMθ of the $(11\bar{2}0)$-Bragg peak of α-alumina as function of ion fluence.

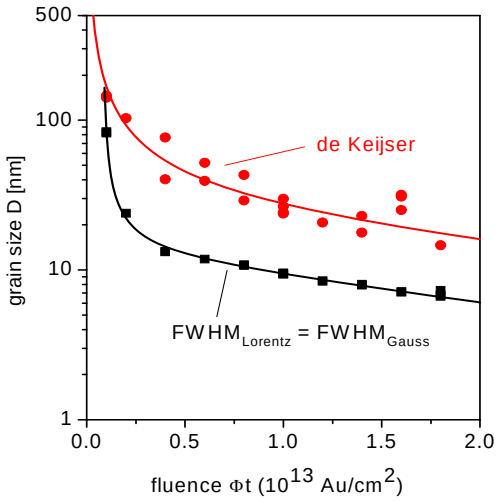

Figure 3: Grain size D versus ion fluence derived from the separation of grain size and strain contributions to FWHMθ. The black curve has been obtained with the usual assumption that the Gaussian and the Lorentzian widths to the Pseudo-Voigt peak widths are equal. The red curve has been obtained by a procedure proposed by de Keijser [1]

[1] de Keijser et al., J. Appl. Cryst. 15(1982) 308-314.

d.severin@gsi.de

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